Aperiodicity-Induced Second-Order Phase Transition in the 8-State Potts Model

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We investigate the critical behavior of the two-dimensional 8-state Potts model with an aperiodic distribution of the exchange interactions between nearest-neighbor rows. The model is studied numerically through intensive Monte Carlo simulations using the Swendsen-Wang cluster algorithm. The transition point is located through duality relations, and the critical behavior is investigated using FSS techniques at criticality. For strong enough fluctuations of the aperiodic sequence under consideration, a second order phase transition is found. The exponents β/ν and γ/ν are obtained at the new fixed point.

The study of the influence of bond randomness on phase transitions is a quite active field of research, motivated by the importance of disorder in real experiments [1]. According to the Harris criterion [2], quenched randomness is a relevant perturbation at a second order critical point when the specific heat exponent α of the pure system is positive.

The analogous situation when the pure system exhibits a first order phase transition was also studied. Imry and Wortis first argued that quenched disorder could induce a second order phase transition [3], and it was shown that in two dimensions, an infinitesimal amount of randomly distributed quenched impurities changes the transition into a second order one [4]. The first large-scale Monte Carlo study of the effect of disorder at a temperature-driven first order phase transition is due to Chen, Ferrenberg, and Landau. These authors studied the 2D 8-state Potts model (which is known to exhibit a first order phase transition when the number of states q is larger than 4 [5]). They first showed that the transition becomes second order in the presence of bond randomness, and obtained critical exponents very close to those of the pure 2D Ising model at the new critical point [6]. On the other hand, drastically different results were obtained for random lattices [7].

The essential properties of random systems are governed by disorder fluctuations. All physical quantities depend on the configuration of disorder, and the study of the influence of randomness requires an average over disorder realisations. Among the systems where the presence of fluctuations is also of primary importance, aperiodic systems have been of considerable interest since the discovery of quasicrystals [8]. They are built in a deterministic way, making any configurational average useless, and their critical properties have been intensively studied (for a review, see Ref. [9]). In layered systems, aperiodic distributions of the exchange interactions between successive layers in the Ising model have been considered [10], leading to unchanged universal behavior or

to modified critical properties, depending on the aperiodic series under consideration. The major result was obtained when Luck, generalizing the Harris criterion to layered perturbations, proposed a relevance criterion for the fluctuating interactions [11]. According to Luck's criterion, aperiodic modulations may be relevant, marginal, or irrelevant, depending on the correlation length exponent ν of the unperturbed system and on a wandering exponent ω which characterizes the fluctuations of the couplings around their average [12]. Systematic studies of the critical properties for irrelevant, marginal, and relevant aperiodic perturbations have then been achieved in the extreme anisotropic limit [13].

In this letter, we report results of Monte Carlo simulations of the two-dimensional 8-state Potts model with an aperiodic modulation of exchange couplings between nearest-neighbor layers. Our aim is to study the effect of such a distribution on the nature of the phase transition. In particular, we ask if the fluctuations are able to induce a second order phase transition. The Hamiltonian of the system with aperiodic interactions can be written

$$-\beta\mathcal{H} = \sum_{(i,j)} K_{ij}\delta_{\sigma_i,\sigma_j} \tag{1}$$

where the spins σ_i, located at sites i, can take the values $\sigma = 1, 2, \ldots, q$ and the sum goes over nearest-neighbor pairs. The coupling strengths are allowed to take two different values $K_0 = K$ and $K_1 = Kr$. They are distributed according to a layered structure *i.e.* the distribution is translation invariant in one lattice direction, and follows an aperiodic modulation $\{f_k\}$ of digits $f_k = 0$ or 1 in the other direction: In layer k, both horizontal and vertical couplings take the same value Kr^{f_k} (Fig. 1). The sequence of digits $\{f_k\}$ is generated through iteration of substitution rules. The Thue-Morse (TM) sequence is obtained by substitutions on digits: $0 \rightarrow \mathcal{S}(0) = 01$, $1 \rightarrow \mathcal{S}(1) = 10$, while the so-called paper folding sequence (PF) is generated through substitutions on pairs of digits: $11 \rightarrow \mathcal{S}(11) = 1101$, $10 \rightarrow \mathcal{S}(10) = 1100$,

original one if one interchanges perturbed and unperturbed couplings $K_1 \leftrightarrow K_0$: $f_s(\tilde{K}_0, \tilde{K}_1; \{f_{L+1-k}\}) = f_s(\tilde{K}_1, \tilde{K}_0; \{f_k\})$. The system being self-dual the critical point, if unique, is exactly given by the critical line $K_{0c} = \tilde{K}_{1c}$ of the usual anisotropic model [14]:

$$(e^{K_c} - 1)(e^{K_c r} - 1) = q. \tag{4}$$

One should mention there that the required symmetry property of the sequences holds for odd iterations in the case of TM, and works in the case of PF if one omits the last digit, which simply introduces an irrelevant surface effect in the simulations.

We performed extensive simulations of $L \times 2L$ lattices ($16 \leq 2L \leq 512$) with periodic boundary conditions in one direction (vertical) and free boundaries in the other ($2L$ columns). The Swendsen-Wang cluster flipping method [15] was used. Between 2×10^5 (smaller lattice sizes) and 6×10^5 (larger lattice sizes) Monte Carlo steps (MCS) per spin were performed (this is always larger than 10^4 times the correlation time, and seems sufficient in order to produce reliable thermal averages).

The order parameter is defined by the majority orientation of the spins [16]:

$$M = \langle m \rangle = \frac{q \rho_{max} - 1}{q - 1}. \tag{5}$$

Here, $\rho_{max} = \langle max_\sigma(\rho_\sigma) \rangle$, where ρ_σ is the density of spins in the state σ and $\langle \ldots \rangle$ denotes the thermal average over the Monte Carlo iterations. The susceptibility is given by $\chi = KV(\langle m^2 \rangle - \langle m \rangle^2)$. Although local ordering mechanisms are not yet clarified in aperiodic systems, we expect a unique transition temperature for all the columns, so we used average quantities in order to reduce fluctuations.

The first task is to identify the order of the transition. For that purpose, we made some preliminary runs at several temperatures first of all in order to confirm numerically the location of the critical point, and then to have a general picture of the phase transition. The examination of the energy autocorrelation time shows that it is diverging in the case of TM sequence, while it seems to remain more or less bounded for PF. It is consistent with a first order transition in the first case, and a second order one for the latter. We have further estimated temperature-dependent effective exponents for the average magnetization and suceptibility. This can be done by comparing the data at two different sizes L and $L' = L/2$: Assuming the following scaling form for the average magnetization $M_L(t) = L^{-\beta/\nu} \mathcal{M}(L t^\nu)$, where $t = |K - K_c|$, we define the quantity [17]

$$X_L(t) = \frac{\ln M_L / M_{L'}}{\ln L / L'}. \tag{6}$$

Close to K_c, this can be expanded in powers of $L t^\nu$, leading to

FIG. 1. Layered aperiodic modulation of the coupling strengths on the square lattice and dual system.

Our particular choice of coupling distribution makes it possible to determine exactly the critical point by duality arguments. Consider a system of L layers with a distribution $\{f_k\}$, made from a succession of vertical-horizontal (V-H) bonds when read from left to right (Fig. 1), and let us write its singular free energy density $f_s(K_0, K_1; \{f_k\})$. Under a duality transformation, the strong and weak couplings K_i are replaced by weak and strong dual couplings $\tilde{K}_i$ respectively. Since a vertical bond on the original lattice becomes horizontal on the dual system, the same V-H bond configuration is recovered for the transformed system when the distribution is read from right to left. One thus gets the same type of system, but a reverse distribution $\{f_{L+1-k}\}$, so that the free energies of the two systems are the same: $f_s(K_0, K_1; \{f_k\}) = f_s(\tilde{K}_0, \tilde{K}_1; \{f_{L+1-k}\})$. The sequences considered here have the interesting property that the reverse distribution corresponds to the

$$X_L(t) \simeq -\frac{\beta}{\nu} + \frac{Lt^\nu}{2\ln 2}\frac{\mathcal{M}'(Lt^\nu)}{\mathcal{M}(Lt^\nu)} + O(L^2 t^{2\nu}) \qquad (7)$$

which defines an effective exponent. As the critical point is approached and in the thermodynamic limit, it evolves towards $-\frac{\beta}{\nu}$. The analogous quantity can be computed for the susceptibility. The results are shown for TM on Fig. 2.
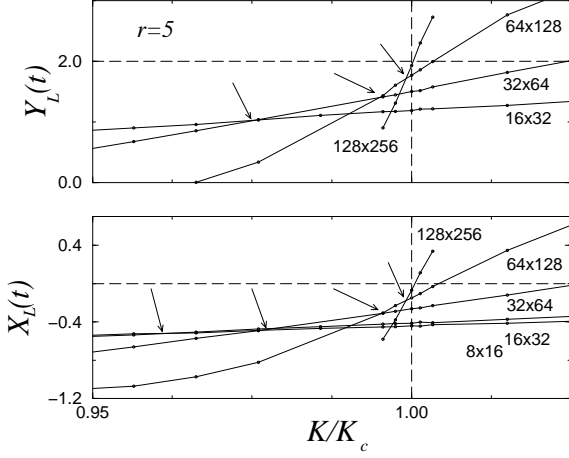

FIG. 2. Temperature-dependent effective exponents for the average magnetization and suceptibility (TM sequence) estimated from the ratios $X_L(t) = \frac{\ln M_L/M_{L/2}}{\ln 2}$ and $Y_L(t) = \frac{\ln \chi_L/\chi_{L/2}}{\ln 2}$ ($K_1/K_0 = r = 5$). The sizes vary from $2L = 16$ to $2L = 256$, and the arrows indicate the crossings between successive sizes which give rough estimates for the critical exponents.

The successive estimates of $\frac{\beta}{\nu} = d - y_t$ and $\frac{\gamma}{\nu} = 2y_h - d$ clearly evolve towards the values 0 and 2, characteristic of a first order phase transition. The scaling dimensions associated to the temperature and magnetic field, y_t and y_h, indeed take a special value equal to the dimension d of the system [18]. In the case of the PF sequence, the behavior is drastically different, and this first analysis does not allow any conclusion.

Once the qualitative description of the phase transition was made, our strategy was to use finite-size scaling (FSS) techniques in order to get more accurate results. We made runs for systems of larger sizes, and in a $L \times 4L$ geometry ($4L$ in the aperiodic direction, going from 8 to 1024), for which we estimated the number of MCS/spin from the preliminary runs. We have moreover studied a periodic system (PS) with alternate couplings K_0 and K_1 (i.e. the same critical point given in Eq. 4), and which is a "first order reference" system. This is illustrated in Fig. 3 where the energy autocorrelation time τ is plotted for the three samples. In the case of TM, τ diverges exponentially as expected for a first order phase transition, although it is always quite small compared to the periodic system. For PF, the data are compatible with a power law with a very small dynamical exponent as

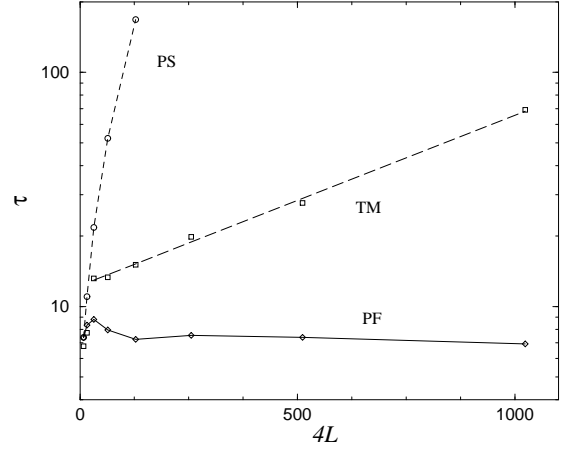expected for cluster algorithm simulations at a second order phase transition.

FIG. 3. Energy autocorrelation time τ at K^c ($r = 5$). For TM, the dashed line is a fit to an exponential behavior.
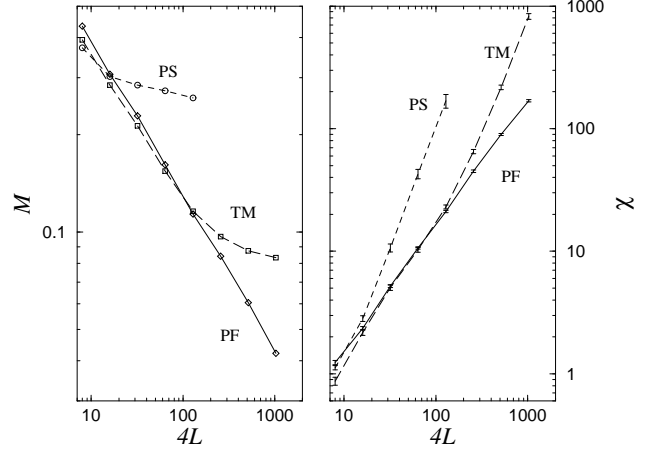

FIG. 4. Log-log plots of M and χ vs L for a periodic reference, and for TM and PF sequences ($r = 5$). For M, error bars are smaller than the symbol sizes.

The crude data for M and χ furthermore show that, in the case of the TM sequence, a cross-over appears between small sizes where the data more or less follow the same behavior than PF, and large sizes where the first order regime analogous to PS is well established (Fig. 4). Certainly, a careful procedure is needed for a reliable determination of the critical exponents. From the log-log curves between $4L_{min}$ and $4L_{max} = 1024$, one determines an effective exponent $x(L_{min})$ for each quantity, then the smaller size is cancelled from the data and the whole procedure is repeated until the three largest sizes only remain. The effective exponent is then plotted against L^{-1} (Fig. 5). The critical exponent is finally deduced from the extrapolation at infinite size. The numerical results are given in Table I. All of them are in agreement with the scaling law $d = 2\beta/\nu + \gamma/\nu$, within the precision of the results.

To summarize, we have shown from numerical simulations that the fluctuations introduced by an aperiodic modulation of exchange interactions is liable to induce a second order phase transition in a system which originally exhibits a first order transition.
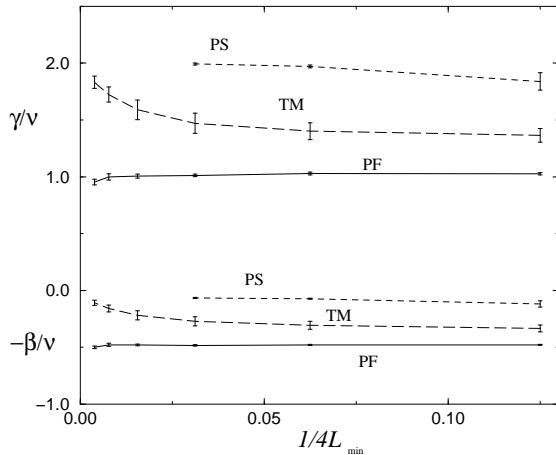

FIG. 5. Effective size-dependent exponents for the two aperiodic sequences ($r = 5$).

TABLE I. Exponents associated to the magnetization and susceptibility for the three examples considered in the text. The uncertainties given there are rough estimations corresponding to the standard deviation for the fit of the data in the whole range of sizes.

	PS	TM	PF
β/ν	0.05 ± 0.03	0.05 ± 0.04	0.48 ± 0.03
γ/ν	1.99 ± 0.08	1.96 ± 0.06	1.01 ± 0.04

From Monte Carlo simulations, we have strong evidences in favor of a second order regime for PF sequence. This type of effect was already known since the work of Imry and Wortis in the case of a random distribution where the fluctuations are unbounded and can be characterized by a wandering exponent $\omega_{\mathrm{rand}} = 1/2$. Here, the same type of behavior is induced by a smoother perturbation, namely by the PF sequence which exhibits only logarithmic fluctuations ($\omega = 0$) while the bounded fluctuations generated by the TM sequence ($\omega = -\infty$) are not strong enough to destroy the first order transition. The same type of problem on a quasicrystal is currently under investigation by Ledue et al and the transition seems, in this case also, to remain of first order [19]. We may thus infer that Luck's criterion can probably be applied to first order phase transition. Here, we can replace ν by $1/d$ [18,20] in the criterion in order to compare thermal fluctuations to those introduced by the distribution of couplings. Luck's cross-over exponent then becomes $\phi = 1 + (\omega - 1)/d$, and the aperiodicity can induce a second order phase transition when $\phi > 0$. This is in agreement with the results of our simulations. We can finally mention that the study of local order parameter is currently under investigation.

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